2-Ethyl-p-xylene 1758-88-9 | DTXSID0061951

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 5.52e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.76e-01

Confidence level: 6.42e-01

Nearest Neighbors from the Training Set

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Terpinolene

Measured: 6.97e-05 Predicted: 6.64e-05

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Limonene

Measured: 7.77e-05 Predicted: 5.10e-05

Image not found

D-Limonene

Measured: 7.77e-05 **Predicted:** 5.10e-05

Image not found

gamma-Terpinene Measured: 6.37e-05 Predicted: 4.78e-05

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5-Ethylidene-2-norbornene **Measured:** 7.40e-05

Predicted: 2.32e-04

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alpha-Pinene

Measured: 1.83e-05 Predicted: 3.40e-05